# OpenCMISS-iron examples and tests used by OpenCMISS developers at University of Stuttgart, Germany

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#### INTRODUCTION 1

This document contains information about examples used for testing OpenCMISSiron. Read: How-to<sup>1</sup> and [1].

- Cmgui files for cmgui-2.9
- Variations to consider
  - Geometry and topology

1D, 2D, 3D

Length, width, height

Number of elements

Interpolation order

Generated or user meshes

quad/hex or tri/tet meshes

- Initial conditions
- Load cases

Dirichlet BC

Neumann BC

Volume force

Mix of previous items

- Sources, sinks
- Time dependence

Static

Quasi-static

Dynamic

Material laws

Linear

Nonlinear (Mooney-Rivlin, Neo-Hookean, Ogden, etc.)

Active (Stress, strain)

- Material parameters, anisotropy
- Solver

Direct

Iterative

Test cases

Numerical reference data

Analytical solution

• A mix of previous items

<sup>1</sup> https://bitbucket.org/hessenthaler/opencmiss-howto

# 1.3 Folder structure

TBD..

# HOW TO WORK ON THIS DOCUMENT

In the Google Doc at https://docs.google.com/spreadsheets/d/1RGKj8vVPqQ-PH0UwMX\_ e9TAzqaYavKi0z0D4pKY9RGI/edit#gid=0 please indicate what you are working on or if a given example was finished

- no mark: to be done
- x: currently working on it
- xx: done

Initials	Full name
СВ	Christian Bleiler
AH	Andreas Hessenthaler
TK	Thomas Klotz
AK	Aaron Krämer
BM	Benjamin Maier
SM	Sergio Morales
MM	Mylena Mordhorst
HS	Harry Saini

 Table 1: Initials of people working on examples, in alphabetical order (surnames).

#### 3 DIFFUSION EQUATION

# 3.1 Equation in general form

The governing equation is,

$$\partial_t \mathbf{u} + \nabla \cdot [\boldsymbol{\sigma} \nabla \mathbf{u}] = \mathbf{f}, \tag{1}$$

with conductivity tensor  $\boldsymbol{\sigma}.$  The conductivity tensor is,

- defined in material coordinates (fibre direction),
- diagonal,
- defined per element.

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

## 3.2.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{2}$$

with boundary conditions

$$u = 0 x = y = 0, (3)$$

$$u = 1$$
  $x = 2, y = 1.$  (4)

No material parameters to specify.

# 3.2.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{5}$$

with boundary conditions

$$u = 0 \qquad \qquad x = y = z = 0, \tag{6}$$

$$u = 1$$
  $x = 2, y = z = 1.$  (7)

No material parameters to specify.

# 3.2.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

• Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

# 3.2.4 Result summary

We use CHeart rev. 6292 to produce numerical reference solutions.

Passed tests: 24 / 24

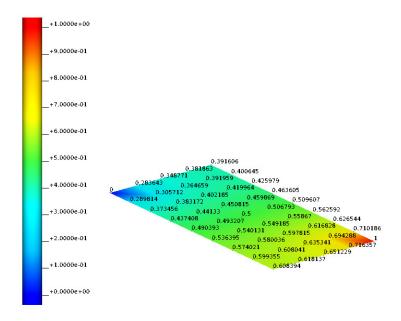


Figure 1: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

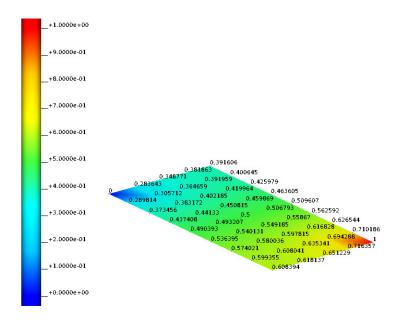


Figure 2: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

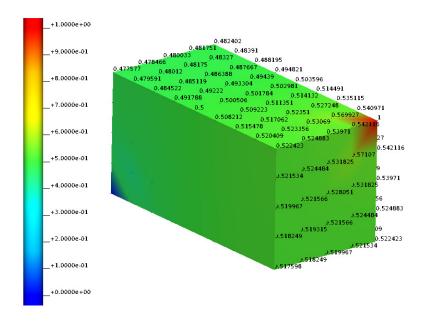


Figure 3: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1 o].

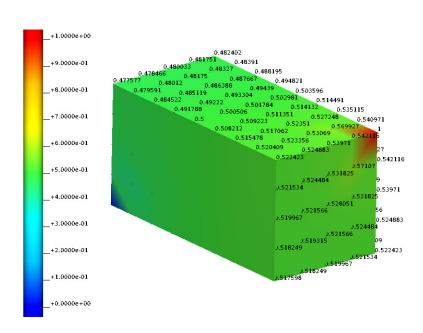


Figure 4: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

# 3.3 Example-0001-u

Example uses user-defined regular meshes in CHeart mesh format and solves a static problem, i.e., applies the boundary conditions in one step.

# 3.3.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{8}$$

with boundary conditions

$$u = 0 x = y = 0, (9)$$

$$u = 1$$
  $x = 2, y = 1.$  (10)

No material parameters to specify.

# 3.3.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{11}$$

with boundary conditions

$$u = 0 \qquad \qquad x = y = z = 0, \tag{12}$$

$$u = 1$$
  $x = 2, y = z = 1.$  (13)

No material parameters to specify.

# 3.3.3 Computational model

Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

```
2.0 1.0 0.0 8 4 0 1 1
2.0 1.0 0.0 2 1 0 2 1
2.0 1.0 0.0 4 2 0 2 1
2.0 1.0 0.0 8 4 0 2 1
2.0 1.0 1.0 2 1 1 1 0
2.0 1.0 1.0 4 2 2 1 0
2.0 1.0 1.0 8 4 4 1 0
2.0 1.0 1.0 2 1 1 2 0
2.0 1.0 1.0 4 2 2 2 0
2.0 1.0 1.0 8 4 4 2 0
2.0 1.0 1.0 2 1 1 1 1
2.0 1.0 1.0 4 2 2 1 1
2.0 1.0 1.0 8 4 4 1 1
2.0 1.0 1.0 2 1 1 2 1
2.0 1.0 1.0 4 2 2 2 1
2.0 1.0 1.0 8 4 4 2 1
```

• Note: Binary uses command line arguments to search for the relevant mesh files.

# 3.3.4 Result summary

We use CHeart rev. 6292 to produce numerical reference solutions.

Passed tests: 24 / 24

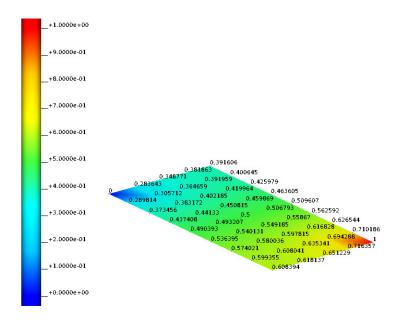


Figure 5: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1

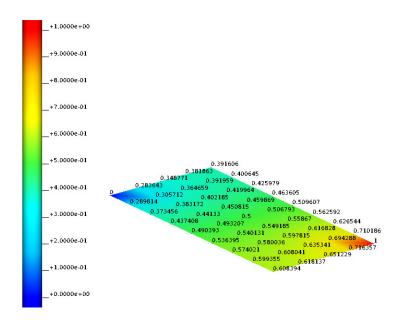


Figure 6: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

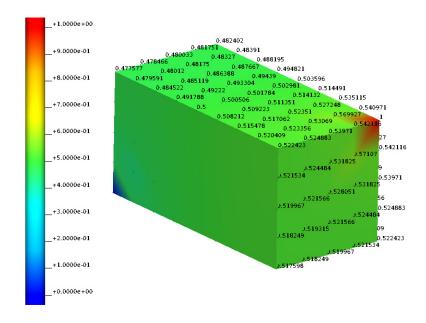


Figure 7: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 1

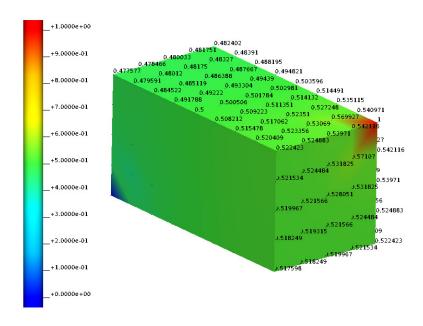


Figure 8: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0].

# 3.4 Example-0002

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

# 3.4.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{14}$$

with boundary conditions

$$u = 15y$$
  $x = 0$ , (15)

$$u = 25 - 18y$$
  $x = 2.$  (16)

No material parameters to specify.

# 3.4.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = \mathbf{0} \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{17}$$

with boundary conditions

$$u = 15y x = 0, (18)$$

$$u = 25 - 18y$$
  $x = 2.$  (19)

No material parameters to specify.

# 3.4.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

# 3.4.4 Result summary

We use CHeart rev. 6292 to produce numerical reference solutions.

Passed tests: 24 / 24

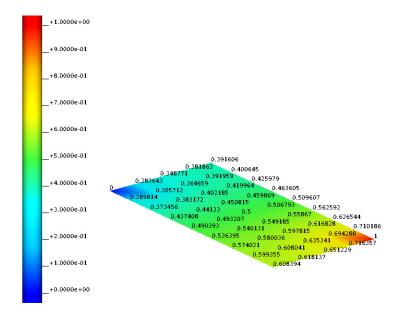


Figure 9: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0].

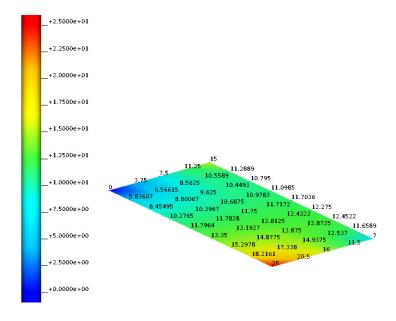


Figure 10: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1  $\,$ o].

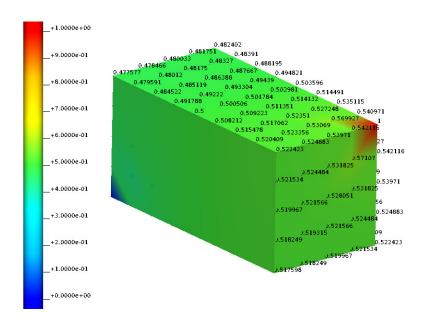


Figure 11: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 10].

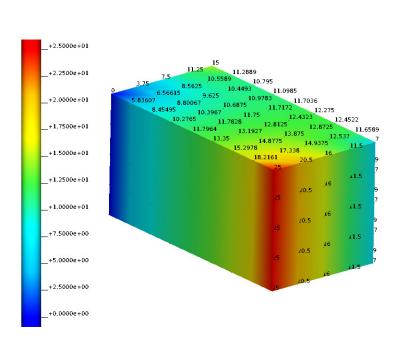


Figure 12: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 o].

# 3.5 Example-0003

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

# 3.5.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{20}$$

with boundary conditions

$$u = 15y \qquad x = 0, \tag{21}$$

$$u = 15y$$
  $x = 0,$  (21)  $\vartheta_n u = 25 - 18y$   $x = 2.$  (22)

No material parameters to specify.

# 3.5.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot \nabla \mathbf{u} = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{23}$$

with boundary conditions

$$u = 15y$$
  $x = 0$ , (24)

$$\partial_n u = 25 - 18y$$
 $x = 2.$ 
(25)

No material parameters to specify.

# 3.5.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

Commandline arguments for tests are:

2.0 1.0 0.0 2 1 0 1 0

2.0 1.0 0.0 4 2 0 1 0

2.0 1.0 0.0 8 4 0 1 0

2.0 1.0 0.0 2 1 0 2 0

2.0 1.0 0.0 4 2 0 2 0

2.0 1.0 0.0 8 4 0 2 0

2.0 1.0 0.0 2 1 0 1 1

2.0 1.0 0.0 4 2 0 1 1

```
2.0 1.0 0.0 8 4 0 1 1
2.0 1.0 0.0 2 1 0 2 1
2.0 1.0 0.0 4 2 0 2 1
2.0 1.0 0.0 8 4 0 2 1
2.0 1.0 1.0 2 1 1 1 0
2.0 1.0 1.0 4 2 2 1 0
2.0 1.0 1.0 8 4 4 1 0
2.0 1.0 1.0 2 1 1 2 0
2.0 1.0 1.0 4 2 2 2 0
2.0 1.0 1.0 8 4 4 2 0
2.0 1.0 1.0 2 1 1 1 1
2.0 1.0 1.0 4 2 2 1 1
2.0 1.0 1.0 8 4 4 1 1
2.0 1.0 1.0 2 1 1 2 1
2.0 1.0 1.0 4 2 2 2 1
2.0 1.0 1.0 8 4 4 2 1
```

# 3.5.4 Result summary

We use CHeart rev. 6292 to produce numerical reference solutions.

current\_run/l2x1x0\_n2x1x0\_i1\_s0/Example.part0.exnode

current\_run/l2x1x1\_n8x4x4\_i2\_s1/Example.part0.exnode

Passed tests: 0 / 24

#### Failed tests:

```
current_run/l2x1x0_n4x2x0_i1_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n8x4x0_i1_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n2x1x0_i2_s0/Example.part0.exnode
                                                             CHeart
current_run/l2x1x0_n4x2x0_i2_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n8x4x0_i2_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n2x1x0_i1_s1/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n4x2x0_i1_s1/Example.part0.exnode
                                                             CHeart
current_run/l2x1x0_n8x4x0_i1_s1/Example.part0.exnode
                                                             CHeart
current_run/l2x1x0_n2x1x0_i2_s1/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n4x2x0_i2_s1/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x0_n8x4x0_i2_s1/Example.part0.exnode
                                                             CHeart
current_run/l2x1x1_n2x1x1_i1_s0/Example.part0.exnode
                                                             CHeart
current_run/l2x1x1_n4x2x2_i1_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x1_n8x4x4_i1_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x1_n2x1x1_i2_s0/Example.part0.exnode
                                                             CHeart
current_run/l2x1x1_n4x2x2_i2_s0/Example.part0.exnode
                                                             CHeart
current_run/l2x1x1_n8x4x4_i2_s0/Example.part0.exnode
                                                            | CHeart
current_run/l2x1x1_n2x1x1_i1_s1/Example.part0.exnode
                                                            | CHeart
\verb|current_run/l2x1x1_n4x2x2_i1_s1/Example.part0.exnode|\\
                                                             CHeart
current_run/l2x1x1_n8x4x4_i1_s1/Example.part0.exnode
                                                             CHeart
current_run/l2x1x1_n2x1x1_i2_s1/Example.part0.exnode
                                                             CHeart
current_run/l2x1x1_n4x2x2_i2_s1/Example.part0.exnode
                                                            | CHeart
```

- Iron  $|_{2} = 27.3358$ - Iron  $|_{-2} = 22.1869$ - Iron  $|_{2} = 19.7449$ - Iron  $|_{-2} = 44.2627$ - Iron  $|_{2} = 37.2776$ - Iron  $|_{-2} = 32.2165$ - Iron  $|_{2} = 27.3358$ - Iron  $|_{-2} = 22.1869$ - Iron  $|_{2} = 19.7449$ - Iron  $|_{-2} = 124.749$ - Iron  $|_{2} = 128.672$ - Iron  $|_{-2} = 143.606$ - Iron  $|_{2} = 94.2619$ - Iron  $|_{-2} = 98.7606$ - Iron  $|_{-2} = 118.047$ 

| CHeart

| CHeart

- Iron  $|_{-2} = 44.2627$ 

- Iron  $|_2 = 37.2776$ 

- Iron  $|_{-2} = 32.2165$ 

- Iron  $|_{-2} = 124.749$ 

- Iron  $|_{2} = 128.672$ 

- Iron  $|_{-2} = 143.606$ 

- Iron  $|_{2} = 94.2619$ - Iron  $|_{-2} = 98.7606$ 

- Iron  $|_{2} = 118.047$ 

Figure 13: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 10].

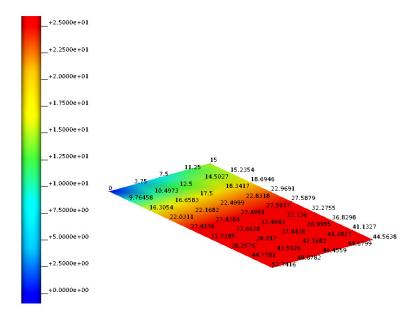


Figure 14: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1  $\,$ o].

Figure 15: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 10].

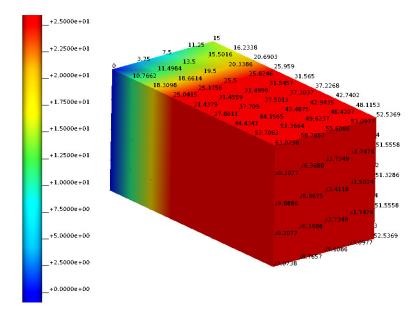


Figure 16: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1  $\,$ o].

# 3.6 Example-0004

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

# 3.6.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot \nabla u = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{26}$$

with boundary conditions

$$u = 2.0e^{x} \cdot \cos(y)$$
 on  $\partial\Omega$ . (27)

No material parameters to specify.

# 3.6.2 Computational model

• Commandline arguments are:

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

interger: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

• Commandline arguments for tests are:

42010

84010

21020

42020

84020

42011

84011

21021

42021

84021

100 50 0 1 0 (not tested yet..)

100 50 0 2 0 (not tested yet..)

100 50 0 1 1 (not tested yet..)

100 50 0 2 1 (not tested yet..)

# 3.6.3 Result summary

We use CHeart rev. 6292 to produce numerical reference solutions.

Passed tests: 10 / 10

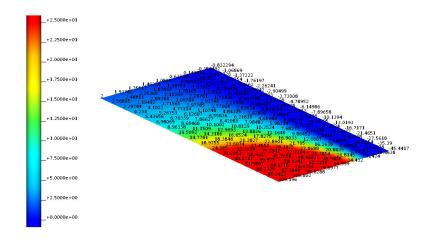


Figure 17: 2D results, iron reference w/ command line arguments [8 4 0 2 0].

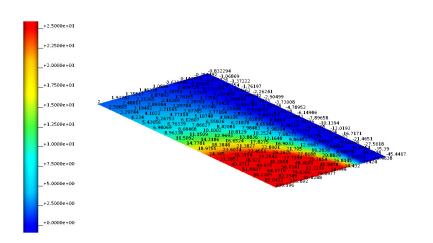


Figure 18: 2D results, current run w/ command line arguments [8 4 0 2 0].

# 3.7 Example-0011

Example uses generated regular meshes and solves a static problem, i.e., applies the boundary conditions in one step.

## 3.7.1 Mathematical model - 2D

We solve the following scalar equation,

$$\nabla \cdot [\sigma \nabla u] = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1], \tag{28}$$

with boundary conditions

$$u = 0 x = y = 0, (29)$$

$$u = 1$$
  $x = 2, y = 1.$  (30)

The conductivity tensor is defined as,

$$\sigma(x,t) = \sigma = I. \tag{31}$$

# 3.7.2 Mathematical model - 3D

We solve the following scalar equation,

$$\nabla \cdot [\boldsymbol{\sigma} \nabla \mathbf{u}] = 0 \qquad \qquad \Omega = [0, 2] \times [0, 1] \times [0, 1], \tag{32}$$

with boundary conditions

$$u = 0$$
  $x = y = z = 0,$  (33)

$$u = 1$$
  $x = 2, y = z = 1.$  (34)

The conductivity tensor is defined as,

$$\sigma(x,t) = \sigma = I. \tag{35}$$

# 3.7.3 Computational model

• Commandline arguments are:

float: length along x-direction float: length along y-direction

float: length along z-direction (set to zero for 2D)

integer: number of elements in x-direction integer: number of elements in y-direction

integer: number of elements in z-direction (set to zero for 2D)

integer: interpolation order (1: linear; 2: quadratic)

integer: solver type (o: direct; 1: iterative)

float:  $\sigma_{11}$ float:  $\sigma_{22}$ 

float:  $\sigma_{33}$  (ignored for 2D)

# • Commandline arguments for tests are:

# 3.7.4 Result summary

We use CHeart rev. 6292 to produce numerical reference solutions.

Passed tests: 24 / 24

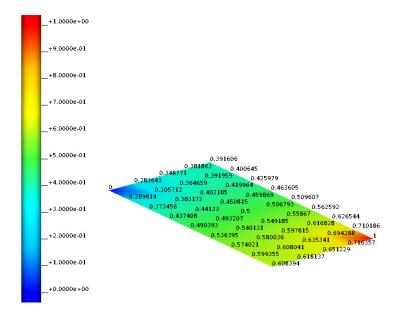


Figure 19: 2D results, iron reference w/ command line arguments [2.0 1.0 0.0 8 4 0 1011].

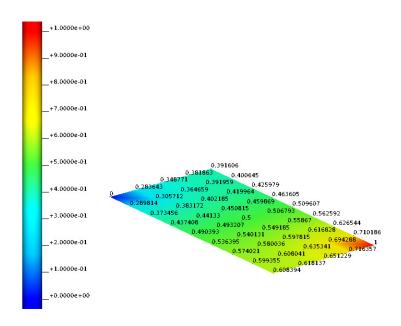


Figure 20: 2D results, current run w/ command line arguments [2.0 1.0 0.0 8 4 0 1 0 1 1].

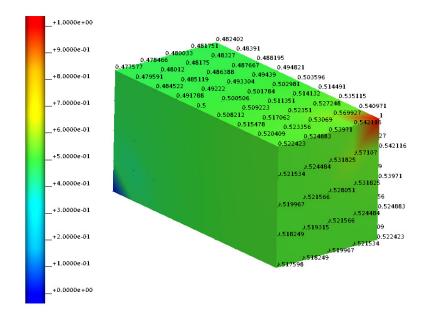


Figure 21: 3D results, iron reference w/ command line arguments [2.0 1.0 1.0 8 4 4 10111].

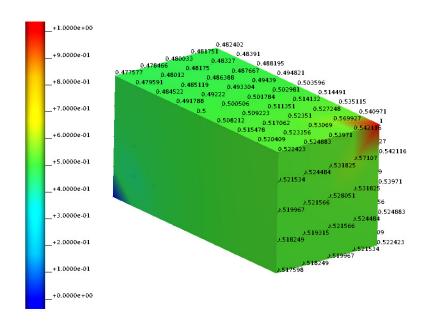


Figure 22: 3D results, current run w/ command line arguments [2.0 1.0 1.0 8 4 4 1 0 1 1 1].

# 4 LINEAR ELASTICITY

4.1 Equation in general form

$$\partial_{tt} \mathbf{u} + \nabla \cdot \mathbf{\sigma}(\mathbf{u}, \mathbf{t}) = \mathbf{f}(\mathbf{u}, \mathbf{t}) \tag{36}$$

# 4.2 Example-0101

# 4.2.1 Mathematical model

We solve the following equation,

$$\nabla \cdot \sigma(\mathbf{u}, \mathbf{t}) = \mathbf{0}$$
  $\Omega = [0, 160] \times [0, 120], \mathbf{t} \in [0, 5],$  (37)

with time step size  $\Delta_{t}=1$  and boundary conditions

$$\dots$$
 (39)

2D: specify thickness, Young's modulus and Poisson's ratio.

# 4.2.2 Computational model

- Length, width, height
- Direct/iterative solver
- Generated/user mesh
- Number of elements
- Interpolation order
- Number of solver steps (time steps, load steps)

# 4.2.3 Results

Figure 23: Results, analytical solution.

# 4.2.4 Validation

CHeart rev. 6328, Abaqus 2017, analytical reference solution, whatever...

Figure 24: Results, Abaqus reference.

Figure 25: Results, iron reference.

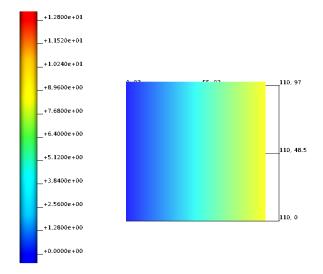


Figure 26: Results, current run.

# 5 FINITE ELASTICITY

# 6 NAVIER-STOKES FLOW

# 7 MONODOMAIN

# 8 CELLML MODEL

# REFERENCES

[1] Chris Bradley, Andy Bowery, Randall Britten, Vincent Budelmann, Oscar Camara, Richard Christie, Andrew Cookson, Alejandro F Frangi, Thiranja Babarenda Gamage, Thomas Heidlauf, et al. Opencmiss: a multi-physics & multi-scale computational infrastructure for the vph/physiome project. Progress in biophysics and molecular biology, 107(1):32-47, 2011.